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THE ROLE OF STATISTICAL METHODOLOGY IN SIMULATION

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ABSTRACT

Statistical methods relevant to both digital and hybrid simulation are presented, using a minimum of formulas. A strategic issue is the ad hoc character of simulation. Statistical methods are surveyed which help to generalize and interpret simulation output data. Moreover statistical tools can show which system variants should be simulated, in order to obtain an understanding of the simulated system configurations. For Monte Carlo simulations some tactical problems are discussed: runlength and variance reduction.

More specifically, the ad hoc character of simulation is mitigated by a formal metamodel (auxiliary model), for which familiar regression analysis is used. The metamodel may include interactions among factors in the simulation experiment, and can be tested for its adequacy. Selecting the values of the input variables is the domain of experimental design. An example demonstrates that seven factors can be examined in only sixteen rather than 2^7=128 runs. Situations with, say, a thousand factors require special screening designs. Requirements for "optimal" designs are briefly discussed.

In stochastic simulation two tactical problems exist: Variance reduction can be achieved through special techniques such as common random numbers, antithetic variates, control variates (regression sampling), importance sampling

(virtual measures). The variance of the simulation output is further affected by the simulation runlength, which leads to questions such as: are we really interested in steady-state behavior, how can we compute a confidence interval for the simulation output, how should we initialize the run, etc.

The survey includes 47 references, many just recently published, and provides references to a number of practical applications of statistical methods.

CONTENTS

1. STRATEGIC PROBLEMS IN SIMULATION

At this conference both digital and hybrid simulation are covered. We hope that the present paper is relevant to the two simulation areas, though we shall emphasize digital simulation, especially discrete-event simulation. In practice, simulation is a method very frequently used to study complex systems[1)]. However, a major practical drawback of simulation is its ad hoc character: After spending much mental effort and computer time to develop, program and run a computer simulation - strictly speaking - the results are valid only for the specific parameter values and structural relationships of the executed simulation program. Changing a parameter or relationship means that the simulation program has to be run again. Nevertheless, such changes are necessary to answer "what if" questions, or to find optimal system configurations, or - not to be forgotten - to establish the sensitivity of the conclusions to specific model assumptions.

Even after a great many simulation runs have been performed, it is difficult to obtain a general understanding of how the simulated system works: During the construction of the simulation model and its program much knowledge about the details of specific system components is acquired. However, insight into the behavior of the total system requires execution of the simulation program. These computer runs yield a mass of data but this mass may turn into a mess. Hence the output data should be summarized by a limited number of measures such as averages, peaks, and correlation coefficients (or spectra). In this way the various system configurations (system variants) are characterized by a few "statistics". Remain the problems of how to determine whether system variants show <u>significantly</u> different outputs, how to discern "patterns" in output changes as system configurations change, and so on.

In this paper we shall present a <u>statistical methodology</u> for generalizing the results of simulation experiments. Because of the survey character of our paper we shall avoid the use of mathematical-statistical formulas as much as possible. As we shall see, the accuracy of the resulting generalizations (metamodels) can be made explicit. Moreover, we shall present a systematic <u>and</u> efficient methodology for the exploration of the great many systems that can be simulated. In Kleijnen (1977) we further described how this methodology fits in the sequence of mental modeling - formal modeling - computer programming - program running - system understanding - optimization - implementation. Before we proceed to the formal presentation of our methodology, we introduce a different problem area in simulation.

2. TACTICAL PROBLEMS IN STOCHASTIC SIMULATION

In Appendix 1 we survey several types of simulation for those readers who do not feel familiar with terms such as discrete-event, stochastic, difference-equation models, etc. Besides the "strategic" problems in simulation models of any type, there are some nagging "tactical" issues, if the simulation is of the Monte Carlo type, i.e., when the program contains stochastic variables generated by means of pseudo-random numbers. Even if we concentrate on a single system configuration with all parameters fixed, we have to decide on the simulation run length. Once we terminate the run, we wish to know the output's accuracy, specified by a statistical confidence interval. The determination of this accuracy may be complicated by serial correlations (autocorrelations) among successive simulation observations so that simple statistical methods are misleading. However, as we shall see, the majority of practical, non-academic simulation experiments can be analyzed without sophisticated statistical analysis techniques. The reason is that most practical studies do not concern long run, steady-state behavior.

Even with modern high-speed digital computers, Monte Carlo simulation may require runs of such lengths that computing time becomes a bottleneck. We might then try to apply special statistical techniques to reduce the variability of the output, and hence the required runlength. This is the area of Variance Reduction Techniques (VRT's), also known as Monte Carlo Techniques, to be discussed in section 6.

3. FORMAL METAMODELS: REGRESSION ANALYSIS

A real-life system can be modeled by means of a simulation model. The relationship between the inputs and outputs of the simulation program (model) can in turn be modeled by a metamodel or auxiliary model, to meet the strategic demands mentioned in section 1. Several types of metamodels are surveyed in Kleijnen (1977): common sense graphical approach, tables with two or three factors, explicit formal metamodels such as the Meisel & Collins (1973) piecewise linear approximations. In this paper, however, we concentrate on linear regression metamodels. The common-sense graphical approach is related to the regression approach, as follows.We may change one factor,say x;observe the resulting output y; repeat this procedure a number of times; plot the (x, y) combinations; fit a curve by hand; and conclude whether x has an important effect on y. The regression approach formalizes this hand-fitting by applying the least squares algorithm. It extends the procedure into multiple dimensions. It further systematizes the various steps, including tests for the importance (significance) of factors together with their interactions, and tests for the adequacy of the fitted regression metamodel. Linear regression analysis has the great advantage of being a familiar technique for most scientists: Regression models have been extensively applied to interpret and generalize experimental results in agriculture, chemistry, engineering, psychology, etc., where these models are also known as Analysis of Variance (ANOVA).Regression metamodels in simulation have been advocated by a few other authors. For instance, Week & Fryer (1977) estimated "main" effects and "interactions" in their job shop simulation study (effects to be defined more precisely below). In their study regression models are further utilized to answer "inverse" questions, i.e., which input values yield fixed, desired output values; see also Kleijnen & Rens (1978), Kleijnen et al. (1978), Koons &

Perlic (1977) and Sherden (1976). The need for some kind of metamodel to assist the more detailed model (simulation, mathematical programming model) has been emphasized by several more authors: Blanning (1974, 1975), Geoffrion (1976), Pegels (1976, p 205).

Note that the variables in a model may be partitioned into decision and environmental variables (factors). Decision (control) variables are under the control of management. Environmental variables are not under management control but do influence the outputs (responses, criteria). In the long run some environmental variables may become controllable, for instance, arrival rates may be influenced by sales promotion. The criterion variables are either satisfied or optimized by a correct selection of the decision variables. The sensitivity of this choice to the assumed environmental factors, must also be investigated.

Let x denote a factor influencing the outputs of the real-world system. The factor may be qualitative or quantitative, continuous or discrete. In Kleijnen (1975, p. 300) it is shown how we can represent a qualitative factor by several dummy variables assuming only the values zero or one. We shall concentrate on qualitative factors (besides quantitative factors) which are studied for only two "levels" or "values". Then this qualitative factor can be represented by a single dummy variable x with the values -1 and +1; see Table 1 below. The response (output) of the real-world system is a time-series. We shall concentrate on a single response variable; for multiple outputs we apply our procedure to each variable separately. In order to compare system configurations, we characterize a whole time path by either a single measure or a few measures: average, standard deviation, correlation coefficients (spectra), slope of a fitted linear trend, peak, etc. Let y_R denote such a measure, characterizing a time path of the real-world system. Hence the response variable y_R is a function of the factors x:

$$y_R = f_1(x_1, x_2, \ldots, x_m) \tag{3.1}$$

The real system is approximated by a simulation model, where $\underline{y}$ is a function of k factors x_j $(j=1,\ldots,k)$, plus a vector of random numbers $\vec{\underline{r}}$. (Vectors and matrices are denoted by $\rightarrow$; stochastic variables are underlined.) Hence the simulation output $\underline{y}$ can be represented as

$$\underline{y} = f_2(x_1, x_2, \ldots, x_k, \vec{\underline{r}}) \tag{3.2}$$

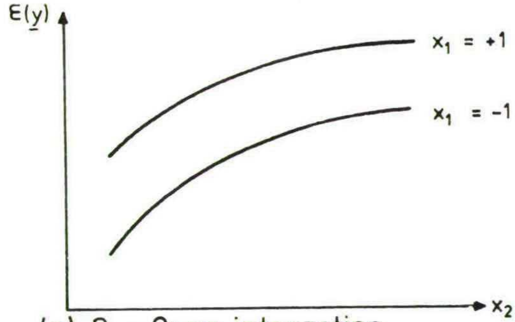
where k is much smaller than the unknown m in eq. (3.1), and $\vec{\underline{r}}$ symbolizes the joint effect of all factors x in eq. (3.1) not explicitly represented in eq. (3.2). The simulation model is specified by a computer program denoted by the function f_2. This model may be approximated in turn by a metamodel (within a specific experimental area E; see below). We propose a metamodel that is linear in its parameters β. This linearity does not mean that the metamodel is linear in its variables x; see eq. (3.5) below. Before we proceed to various specific metamodels we observe that the metamodel approach also applies when no sampling is used so that $\vec{\underline{r}}$ in eq. (3.2) vanishes; see Appendix 1 for the various simulation types.

The simplest metamodel to express the effects of the k factors would be:

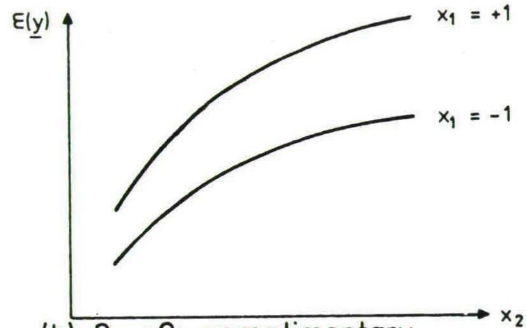
$$\underline{y}_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_k x_{ik} + \underline{e}_i \qquad (i=1,\ldots,N) \tag{3.3}$$

where in simulation run i (observation i) factor j has the value x_{ij} $(j=1,\ldots,k)$ and $\underline{e}_i$ represents the noise (disturbance, error) in the metamodel which is assumed to have zero expectation. Such a simple metamodel implies that a change in x_j has a constant effect on the expected response, $\mathcal{E}(\underline{y})$:

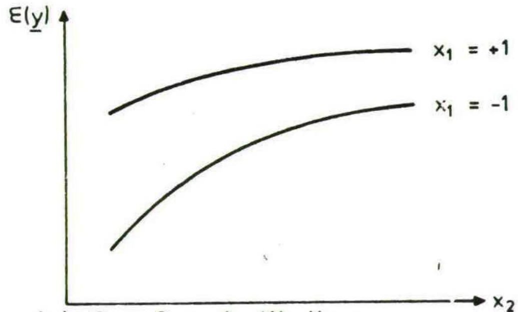
$$\frac{\partial[\mathcal{E}(\underline{y})]}{\partial x_j} = \beta_j \qquad (j=1,\ldots,k) \tag{3.4}$$



(a) $\beta_{12} = 0$: no interaction



(b) $\beta_{12} > 0$: complimentary



(c) $\beta_{12} < 0$: substitution

FIG. 1 Interactions

A more general metamodel postulates that the effect of factor j also depends on the values of the other factors j' ($j' \neq j$). This can be formalized as in eq. (3.5) where for illustration purposes we take k = 3:

$$\underline{y}_i = \beta_0 + (\beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3}) + $$
$$+ (\beta_{12} x_{i1} x_{12} + \beta_{13} x_{i1} x_{13} + \beta_{23} x_{i2} x_{i3}) + \underline{e}_i$$
$$(i=1,\ldots,N) \qquad (3.5)$$

Here the parameters (coefficients) β_{12}, β_{13} and β_{23} denote <u>interactions</u> between the factors 1 and 2, 1 and 3, and 2 and 3 respectively. A graphical illustration of interaction in the case of two factors (k=2), is shown in FIG. 1. In case (a) of FIG. 1 the curves are parallel, i.e., the effect of x_2 on $\mathcal{E}(\underline{y})$ does not depend on the level of x_1. In case (b) the interaction coefficient β_{12} is positive. Hence the two factors are <u>complimentary</u>, i.e., as x_2 increases the increase in $\mathcal{E}(\underline{y})$ is stimulated when the increase of x_2 is accompanied by an increase in x_1. In case (c) the marginal output of x_2 is much smaller when more of x_1 is available which can be substituted for x_2.[2)] The need to consider interactions among factors when analyzing simulation results, has been emphasized by Koons & Perlic (1977) in their case-study of a steel plant.

If all factors are quantitive, continuous variables, then we add "purely quadratic" effects β_{jj} to eq. (3.5). This yields

$$\underline{y}_i = \beta_0 + \sum_{j=1}^{3} \beta_j x_{ij} + \sum_{j<j'}^{2} \sum^{3} \beta_{jj'} x_{ij} x_{ij'} + $$
$$+ \sum_{1}^{3} \beta_{jj} x_{ij}^2 + \underline{e}_i \qquad (3.6)$$

which represents the Taylor series expansion of eq. (3.2), cut off after the second-degree terms. For an application of eq. (3.6) we refer to Koons & Perlic (1977, p.7). We feel that in practice it is rare that all factors are quantitative, so that we shall concentrate on the metamodel with k main effects β_j, k(k-1)/2 two-factor interactions $\beta_{jj'}$ and the general (overall) mean β_0. In symbols:

$$\underline{y}_i = \beta_0 + \sum_{j=1}^{k} \beta_j x_{ij} + \sum_{j<j'}^{k-1} \sum^{k} \beta_{jj'} x_{ij} x_{ij'} + \underline{e}_i \qquad (i=1,\ldots,N) \qquad (3.7)$$

We start by assuming a metamodel, such as eq. (3.7), but next we test statistically whether this assumption was realistic! Two statistical tests can be used:

(1) Generate some new observations $\underline{y}$ using the simulation model. Use the familiar Student t-statistic to compare these observations $\underline{y}$ to the predicted value $\hat{\underline{y}}$ based on the regression metamodel which was estimated from the old observations.[3)]

(2) A so-called lack-of-fit F-statistic can be computed which compares the "mean residual sum of squares" to the "pure error".

For details on both approaches we refer to Kleijnen et al. (1978).

If the assumed metamodel turns out to be unreasonable, we have several alternatives:

(1) Make the metamodel more complicated by adding terms such as three-factor interactions. If $\underline{y}'$ is a shorthand notation for $\underline{y}$ in eq. (3.5), then we may expand (3.5) to

$$\underline{y}_i = \underline{y}_i' + \beta_{123} x_{i1} x_{i2} x_{i3} \qquad (3.8)$$

The intuitive interpretation of three-factor interactions is difficult. Moreover these interactions mean additional parameters. Hence we prefer the next alternative.
(2) Look for transformations of x. For instance, if $\underline{y}$ denotes waiting time, and x_1 and x_2 denote mean arrival and service rate, then the transformation $x' = x_1/x_2$ implies that the original metamodel

$$\underline{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \underline{e} \tag{3.9}$$

is replaced by a new metamodel:

$$\underline{y} = \gamma_0 + \gamma_1 x' + \underline{e}' \tag{3.10}$$

We strongly recommended to look for such transformations, from the very beginning of the study! The transformation can be based on the relevant theory, for instance, queuing analysis in the above example. A popular transformation in econometrics is $x' = \log x$, $\underline{y}' = \log \underline{y}$, so that the parameters β represent elasticity coefficients. A more complicated example is provided by Yen & Pierskalla (1977). A simple transformation is also utilized in the case study by Kleijnen et al. (1978).
(3) Reduce the experimental area E. This option limits the generality of our conclusions. However, if the only purpose of the metamodel is to find the optimum x-values, then a small area E can be used, a metamodel fitted, and the direction of better x-values determined. See Montgomery & Bettencourt (1977) for details on this so-called Response Surface Methodology (RSM). For a bibliography we also refer to Kleijnen (1975).

Note that, after we have used the metamodel to meet the demands of sensitivity analysis, optimization, and so on, we can return to the original simulation model to study the system behavior in detail, e.g., to study its dynamics.

The parameters β in the above equations can be estimated and tested for their significance, using the familiar technique of regression analysis, applying either Ordinary or Generalized Least Squares; see e.g. Draper & Smith (1966). Least Squares is also summarized in Kleijnen et al. (1978).

5. EXPERIMENTAL DESIGN

As we mentioned in section 1 parameters, variables, and structural relationships in the simulation model are changed in order to perform sensitivity analysis, answer what-if questions, do optimalization studies, etc. "Infinitely" many system configurations (system variants or briefly systems) may be of potential interest. Even with modern fast computers simulating all system variants is out of the question. The problem of selecting a limited number of system variants for actual simulation evaluation can be solved by means of statistical methods known as experimental design methodology. Experimental design theory has been developed since the 1920's and has been widely applied to experiments in agriculture, chemistry, etc. Unfortunately, its application to the management and social sciences is still in its infancy. The reason is that in sociotechnical systems the scientific design of experiments is difficult and expensive (disruption of the organization). However, in a simulation model of such a social system, the experimental factors are completely under the scientist's control, so that experimental design methods become relevant. Let us consider some simple examples.

If we study the effects of just a few factors, say three, then we may start by letting each factor assume only two "values" or "levels" denoted by $x = +1$ and $x = -1$ respectively, and evaluating the responses at all combinations, i.e., at $2^3 = 8$ combinations. (Remember that one factor combination specifies one system variant to be simulated.) But, if we are willing to assume that the "first order" model of eq. (3.3) is adequate, then we need to estimate only four effects, namely β_0, β_1, β_2 and β_3. Before reading on, the reader is challenged to specify his own selection of the x-combinations! Next he may compare his selection to Table 1. This table is constructed using a "trick" developed in experimental design theory: The last column x_3 is obtained by multiplying the corresponding elements in the x_1 and x_2 columns. Such tricks certainly become necessary as the number of factors increses, since in that case the number of combinations N grows dramatically. For instance, for seven factors we have $N = 2^7 = 128$. Table 2 displays a design for seven factors[4]: If we assume a first order model, then only the first eight combinations need to be evaluated, in order to estimate β_0, β_1, ...,β_7. If we leave open the possibility that such a metamodel is inadequate, then the next eight combinations should also be evaluated. The first eight combinations form a so-called 2^{7-4} fractional factorial design of "resolution III". The sixteen combinations together form a 2^{7-3} fractional factorial of "resolution IV", and can give us an idea of the importance of interactions besides main effects; see Kleijnen (1975) for more details. Observe that a design matrix such as Table 1 also specifies the cross-products x_1x_2, x_1x_3 and x_2x_3 in eq. (3.5).

The above phase of the investigation may be preceded by a pilot or scréening phase. In the latter stage a great many, say a hundred or a thousand factors may be conceived of, but hopefully only relatively few are really important. Detecting these important factors can be based on special experimental designs: group-screening, random designs, etc. Random designs (randomly selected factor combinations) were applied in a water-resource simulation; Maass et al. (1962). Group-screening [5] was utilized in the simulation of computer systems - see Schatzoff & Tillman (1975) - but applications of this class of designs are extremely rare. Nevertheless we imagine that it is quite common to have simulation models

Table 1

Experimental Design for Three Factors

Combination	x_1	x_2	x_3 $(= x_1x_2)$
1	+1	+1	+1
2	-1	+1	-1
3	+1	-1	-1
4	-1	-1	+1

Table 2

Experimental Design for Seven Factors

Combination	x_1	x_2	x_3	x_4	x_5	x_6	x_7
1	-	-	-	+	+	+	-
2	+	-	-	-	-	+	+
3	-	+	-	-	+	-	+
4	+	+	-	+	-	-	-
5	-	-	+	+	-	-	+
6	+	-	+	-	+	-	-
7	-	+	+	-	-	+	-
8	+	+	+	+	+	+	+
9	+	+	+	-	-	-	+
10	-	+	+	+	+	-	-
11	+	-	+	+	-	+	-
12	-	-	+	-	+	+	+
13	+	+	-	-	+	+	-
14	-	+	-	+	-	+	+
15	+	-	-	+	+	-	+
16	-	-	-	-	-	-	-

with a great many parameters and variables, which could benefit from group-screening designs. Several types of screening designs are evaluated in Kleijnen (1975 b).

Let us briefly evaluate the designs derived in the statistical design literature. The traditional, "common sense" approach is to change one factor at a time: ceteris paribus approach. We proposed to change several factors simultaneously; see Tables 1 and 2. Such factorial designs (full or fractional) are more efficient, i.e., they yield more accurate estimators of the factor effects, and they provide estimates of possible interactions among factors. Some problems, however, remain: Specific designs such as 2^{k-p} designs, and the concomittant regression analysis yield "optimal" results only under certain statistical assumptions such as constant variances. How robust are these optimality properties and what are the alternatives? Ad hoc optimal designs specified by computer, generalized least squares, robust estimation procedures, etc. are surveyed in Kleijnen et al. (1977). Designs such as in Tables 1 and 2 may be evaluated against the following requirements:

(1) A small number of runs N: Obviously, to estimate q parameters it is necessary that $N \geq q$. However, N may be much smaller than 2^k, for instance, in Table 2 N = 16 whereas $2^7 = 128$.

(2) Maximum statistical accuracy, given the number of runs: If the classical statistical assumptions hold, then the accuracy requirement is satisfied by choosing an orthogonal design; otherwise the selection of the design matrix poses a problem not yet solved. Note that Tables 1 and 2 do yield orthogonal columns.

(3) Providing a measure for the adequacy of the fitted metamodel: If $N > q$ then a lack-of-fit F-statistic exists. If besides the N observations we have one or more runs, not used in the estimation of the parameters, then "validation" of the model is possible, using a t-test.

(4) Desirable "confounding" (bias, alias pattern): If not all factor effects can be estimated from N runs only, the main effects should be biased by high order effects (say,

three-factor interactions), not by other main effects. The designs derived by experimental design theory immediately show how effects are biased by other effects.

(5) Flexibility of the design: Unfortunately, in many standard designs the number of runs N is restricted to a power of two (2^{k-p} designs) or a multiple of four. Fortunately, it remains possible to start with only a small number of runs, to test the results, and to proceed to a larger design that yields more detailed estimates, so-called sequentialized designs; see Kleijnen (1975, pp. 344-345, 367-370).

(6) Numerical inaccuracy caused by an ill-conditioned matrix $\vec{X}$: An orthogonal matrix $\vec{X}$ eliminates such problems. When using normalized variables (between -1 and +1) we should not forget to translate the estimated effects back into the original effects; see Kleijnen et al. (1978).

Note that, if the assumed metamodel turns out to be completely misleading, then the "optimal" properties of the experimental design break down. For instance, if the interaction between the factors 1 and 2 in Table 1 is actually important then we cannot estimate the main effect of factor 3 since it is completely confounded with that interaction. To reduce the possibility of such events, preliminary experimentation and analysis is necessary; see also Kleijnen (1975, pp. 391-393) and Kleijnen et al. (1978).

In conclusion, the literature on experimental design is overwhelming, and still growing! As a sample we mention the recent textbook Daniel (1976). In Kleijnen (1975, pp. 287-450) we have given a selection from the vast literature, tailored to the needs of the simulation practitioner: The focus is on simple designs such as 2^{k-p} designs, excluding sophisticated designs such as "partially balanced incomplete block designs". Excluded are techniques not needed in simulation, e.g., randomization and blocking are needed in case of incomplete control over the experiments as in areas outside simulation.

5. SUMMARY OF STRATEGIC PROBLEM

Formal metamodels are a useful technique for generalizing and interpreting simulation output. An important aspect of this interpretation is the concept of factor interaction. Efficient exploration of the simulation space requires an experimental design. Work on statistical designs is abundant but unfamiliar to the majority of simulation practitioners. Our experience is that the necessary statistical techniques can be learned without too many problems. Observe, however, that these techniques alone cannot solve the problem for the scientist! The models and hypotheses to be evaluated by the statistical techniques, have to be provided by management or by other, non-statistical specialists. The use of the techniques leaves much freedom: freedom of interpretation, choice of significance levels α, etc. Hence an automated application of techniques is impossible. Moreover, all statistical techniques are based on certain statistical assumptions such as constant variances, which are not satisfied in practice. It remains a challenge to develop more general and robust techniques. In the mean time, the practioner must use his judgement in the selection and use of his statistical tools. Nevertheless we feel that these tools result in a more efficient exploration of the experimental area, and in a better idea of both the limitations and the generalizations of the simulation experiment. In this way, one important drawback of simulation is mitigated, namely its ad hoc character. For an elaborated case study using a variety of statistical techniques, we refer to Kleijnen et al. (1978).

6. TACTICAL PROBLEMS IN STOCHASTIC SIMULATION: VARIANCE REDUCTION

In the following sections we shall focus on problems arising when simulating one specific system configuration, i.e., a single factor combination. The problems we shall discuss arise in stochastic simulation models only: runlength determination in relation to estimation of the variances of the simulation response, and reduction of that variance through special statistical techniques, so-called Variance Reduction Techniques (VRT's).

Though we devoted a doctoral dissertation to the issue of VRT's - see Kleijnen (1975, pp. 105-285) - over the years we have grown very pessimistic as to the practicality of such techniques. Note that computer time can be saved (and variance reduced through additional runs) by other devices than VRT's, e.g., more efficient random number generation, faster sampling procedures, better software. In Kleijnen (1975, pp. 105-285) we discussed six VRT's in detail including some applications, and provided references to many more techniques. Four VRT's will be briefly discussed in the present paper.

(1) Common random numbers

A system configuration may be simulated using the same random number seed as in the other system variants, so that systems are compared "under the same circumstances". This is the only VRT often applied by practitioners. Kleijnen (1975) discussed the practical complication of synchronizing random number streams per type of stochastic process. A complication overlooked by most practitioners, is that the analysis of the simulation results gets more difficult when the outputs become dependent, e.g., ordinary least squares assumes independent responses y. The following VRT is (nearly) as simple as the use of the same random numbers, but does not complicate the analysis.

(2) Antithetic variates

Suppose the first run of a specific system configuration is generated from the random number stream r_0, r_1, r_2,... and yields the result y_1. Then the "antithetic" run is generated from the complements $1-r_0$, $1-r_1$, $1-r_2$,... and yields y_2. The idea is, that when y_1 happens to undershoot its expected value, then y_2 is expected to overshoot that value. (Example: In run 1 most r's happen to be small, so that service times are short, and waiting times are short. In run 2 most r's are large, etc.) Statistically speaking, $\underline{y}_1$ and $\underline{y}_2$ are conjectured to be negatively correlated, so that the variances of their average decreases. The statistical analysis remains simple since it can be based on the n/2 averages of the antithetic pairs (y_1, y_2) (y_3, y_4), ..., (y_{n-1}, y_n). Kleijnen (1975a) discussed the surprising fact that it is not necessarily optimal to combine antithetic variates and common random numbers when comparing two system variants. Recently Schruben & Marjolin (1977) investigated the joint application of these two VRT's when investigating N system variants in an experimental design. They found that applying either common random numbers only, or a specific combination[6)] of common and antithetic random numbers, reduced the estimated variance by 80% compared to independent random number streams.

(3) Control variates or regression sampling

During a simulation run we may keep track of the average value $\hat{\mu}$ of the input variable, say, interarrival time. Note that the expected value μ is known, since we sample the input from a known distribution function. If we wish to estimate, say, average waiting time η for a specific average input value μ, then we may correct our estimate via the regression model

$$\underline{y}_i = \beta_0 + \beta_1 \cdot \underline{x}_i + \underline{u}_i \qquad (i=1,\ldots,n) \qquad (6.1)$$

where $\underline{y}_i$ is the average waiting time of run i, $\underline{x}_i$ is the average interarrival time ($\underline{x} \equiv \underline{\hat{\mu}}$) of run i, $\underline{u}$ is an error term, and the β's are regression coefficients. Hence

$$\hat{\underline{y}}_{\mu} = \hat{\underline{\beta}}_0 + \hat{\underline{\beta}}_1 \cdot \mu$$

$$= \bar{\underline{y}} + \hat{\underline{\beta}}_1 (\mu - \bar{\underline{x}}) \qquad (6.2)$$

where $\bar{\underline{y}}$ is the "crude" average response of the n simulation responses $\underline{y}_i$, which is corrected by the "control variable" $\underline{x}$. We found a variance reduction factor of 3.84 in a case study, a telephone exchange simulation; however, the estimator (6.2) does involve some statistical complications as shown in Hopmans & Kleijnen (1977).

(4) Importance sampling and virtual measures

There is one class of systems that might benefit very much from variance reduction, viz., systems where we are interested in "rare events" such as "excessive" waiting times, inventory stockouts, etc. During most of the simulation run nothing of interest happens. A VRT especially relevant for such systems seems importance sampling (IS), and a closely related technique known as "virtual measures". These techniques sample more frequently that part of the time path during which rare events tend to occur more frequently (and correct for that oversampling). In a recent case study we applied this idea to a telephone-exchange simulation studying blocking probabilities (all lines occupied). Unfortunately, the practical results were very disappointing; see Hopmans & Kleijnen (1978).

7. TACTICAL PROBLEMS: RUNLENGTH

Under the heading "runlength" we shall discuss a set of related questions such as:

- How long to continue the simulation run?
- How to start the run (initialization)?
- How often to replicate (repeat) the run with different random number seeds?
- How accurate is the estimated response (confidence intervals)?

An important remark to start with, is that in practical, as opposed to academic, simulations these questions can often be answered using only elementary statistical techniques, such as t-statistics.

In practice simulation models are usually terminating, i.e., the simulation run is stopped when a specific event occurs. Simple examples are:

(1) In studying maintenance policies the simulation run may end when the equipment (say, a computer) breaks down. A new run starts with a "perfect" piece of equipment.

(2) A queuing (waiting-line) system such as a bank or hospital clinique, is closed at 5 P.M. (critical event). The new run corresponds with a new day, starting in the "empty" state.

(3) A corporate simulation model can be utilized to examine a policy's effect on profit over the next three months (planning horizon). The simulation run of three months is repeated for different policies (what-if), starting each run from the most recent "situation" (system state). Note that corporate models are often non-stochastic.

(4) Queuing systems that never close down are, e.g., a telephone exchange and a highway crossing. Such systems may be simulated to see whether the system configuration can handle peak traffic. As soon as the rush hour is over (critical event, defined fuzzily), the simulation run is terminated. A next run starts from a pre-rush-hour situation. The same or different random numbers (see section 6 on variance reduction) may be utilized in that next run, to study the sensitivity to the starting conditions (and to the random number seed). Example 4 seems to be the most problematic example, and may merit additional research.

In the above examples there is no interest in steady-state responses! Steady-state (stationary, equilibrium, long-run) behavior means that the distribution function (probability law) does not change over time. In the above examples, however, start-up and end effects are part of the relevant output. Each simulation run yields a single observation on the output, say, the average waiting time or the total profit. (The relevance of transient behavior is also emphasized in Fox (1978) and Lam & Pedersen (1977).) If the simulation is stochastic, more accurate estimates can be obtained by repeating (replicating) the run with different random numbers (possibly antithetic, see section 6). The statistical analysis is straightforward for terminating systems. For example, if $\underline{y}_i$ denotes average waiting time in run $i(i=1,\ldots,n)$, then its standard deviation (standard error) is estimated by

$$\underline{s}_y = \{\sum_{i=1}^{n} (\underline{y}_i - \bar{\underline{y}})^2/(n-1)\}^{\frac{1}{2}} \tag{7.1}$$

A confidence interval for the expected value η can be based on the Student t-statistic:

$$P\{\eta \leq \bar{\underline{y}} + t^{\alpha}_{n-1} \cdot \underline{s}_y/\sqrt{n}\} = 1-\alpha \tag{7.2}$$

For an application we refer to Kleijnen (1978) where Chapter IX concerns a simulation experiment with an IBM management game, used to study the financial benefits of accurate information.

If the confidence interval in (7.2) turns out to be too long, we may increase the accuracy of the average simulation output $\bar{\underline{y}}$ by generating additional runs. The total number of runs for a fixed length c of the confidence interval, should be

$$\underline{n} = \{t^{\alpha}_{n-1}/c\}^2 \cdot \underline{s}^2_y \tag{7.3}$$

For additional comments[7)] on such a sequential approach we refer to Kleijnen (1975).

In the simulation literature most attention is focussed on steady-state behavior. Such behavior is primarily of academic interest: Simulation is used by many academics in the study of analytic models such as queuing models; see the examples in Ignall et al. (1978). Transient behavior of such models is difficult to analyse - Kotiah(1978), Liittschwayer & Ames(1975) - so that most academic studies concentrate on steady-state(limiting) behavior. Simulations with the (practical!) aim of assisting such theoretical studies, are confronted with serious problems: Should the simulation be continued or should replicated runs be used? Replicated runs yield independent observations (on, say, steady-state average waiting time) but each run creates an initialization problem (transient behavior). A single prolonged run consists of many dependent individual responses: autocorrelation or serial correlation problem. For instance, if customer i has to wait "very" long (longer than average) then the next customer probably has to wait longer too (positive correlation). Elementary statistical techniques assuming independence, are misleading in that case. The variance of the average of the continued run $\bar{\underline{w}}$ based on m autocorrelated individual observations $\underline{w}$ is given by:

$$\mathrm{var}(\bar{\underline{w}}) = \{1+2\sum_{j=1}^{m}(1-\frac{j}{m})\rho_j\}\sigma_w^2/m \qquad (7.4)$$

where ρ_j is the autocorrelation between $\underline{w}_t$ and $\underline{w}_{t+j}$, and σ_w^2 is the variance of an individual observation $\underline{w}$. If the w's were independent ($\rho_j = 0$), then the variance of their average would reduce to the familiar expression σ_w^2/m. So the autocorrelation ρ inflates the variance of the average, and should not be ignored. Several approaches are possible.

(1) Repeated runs

As mentioned above, replicated runs result in independent observations so that the analysis becomes simple. However, each run is confronted with the initialization problem. References on this approach and its alternatives will be given below.

(2) Prolonged run with (nearly) independent subruns of fixed length

Assume that the serial correlation among the individual observations decreases as the observations are farther apart. Divide the total run (usually after removing the initial phase as in approach 1 above), into subruns of fixed length. Though the first "few" observations of a subrun still depend on the last "few" observations of the preceding subrun, the subrun *averages* will be independent, practically speeking, provided the subrun length is "long enough".Therefore a subrun length may be selected intuitively; the autocorrelation among subrun averages be tested (through the estimated autocorrelation coefficient of lag 1 or through von Neumann's ratio); if the autocorrelation is too high (empirical threshold) then the subrun length is increased, etc. A recent paper on this approach is Law & Carson (1977). In practice, approach 2 is often followed, but with the subrun length being selected purely intuitively. Relying on intuition alone seems dangerous: Analytical results for simple queuing systems demonstrate that for heavy traffic individual observations remain correlated over surprisingly long lags. On the other side, overestimating the autocorrelation means that the subruns are too long, so that too few subruns remain.[8)]

(3) Prolonged run without subrun distinction, but with estimated individual autocorrelations

Eq. (7.4) displayed the effects of the autocorrelation coefficients ρ_j ($j=1,2,...$) among the individual observations. In the sixties Fishman and Kiviat, at that time with the RAND Corporation, published several reports in which the variance of the average simulation output was based on the estimation of those coefficients ρ_j (or their Fourier transformations: spectral analysis). For a recent discussion we refer to Clark (1977). In practice this approach has never been popular: cumbersome estimation of the ρ's; difficult selection of m (the number of ρ's to be incorporated).

(4) Prolonged run with truly independent subruns based on the renewal property

Both Iglehart and Fishman have pioneered the application of the renewal or regenerative property shown by many simulated systems. Consider a queuing system that has become empty. Then the next history (timepath) is independent of the past history! Consequently, the total run can be divided into subruns, each subrun starting as soon as the system has become empty. In contrast to the subruns of fixed length (approach 2) the new subrun definition creates subruns of stochastic lengths: when does the system return to the empty state? These subruns are exactly independent! The estimation of the total run's average involves some statistical complications: ratio estimators for point estimation, jackknifing for confidence intervals, etc. Estimating quantiles[9)] such as the 90%-point, involves some more problems; see Seila (1978) and also Coppus et al. (1977). Percentiles (e.g., the probability of queue-sizes exceeding the waiting room capacity) are studied by Fishman & Moore (1977). However, it is our experience (with graduate students in management science and econometrics) that these statistical complications are easily overcome. In general, any Markov system shows the renewal property. However, practical problems remain: The renewal state may occur so infrequently that too few subruns result; see Hopmans & Kleijnen (1978) for an example. Approximative renewal states may then be formulated; see Gunther (1975). A recent textbook on the renewal approach is Crane & Lemoine (1978); see also Fishman (1978). Since we feel that this is an important technique for the exact analysis of steady-state (academic) simulations, we mention some more applications: Lavenberg & Slutz (1975) and Schwetman & Bruell (1976). A case study (a simple time sharing system) comparing this approach to replicated runs (approach 1) is provided by Sargent (1977).

The initialization problem was mentioned several times in the present section. Remember that this problem exists primarily in steady-state, academic simulations. An example of initialization in a practical simulation for planning purposes, is provided by Jain (1975, p. 85): "at the start of a simulation the model represents the actual state of the machine shop." Note further that in the renewal approach to steady-state simulations, there is no start-up problem: observations can be collected immediately when the simulation starts in the renewal state (e.g. the empty state). In the other three approaches the transient phase does pose a problem: Usually initial observations are thrown away though this is not necessarily optimal. Recently Wilson & Pritsker (1977) investigated a variety of heuristics, and concluded that it seems best to start the simulation run in the most likely stationary state, and to retain all observations (transient and steady-state).

8. MISCELLANEOUS STATISTICAL PROBLEMS

In the above sections we concentrated on those statistical problems we thought to be most relevant in the analysis and design of simulation experiments. In the present section we briefly discuss some remaining issues.

(1) Multivariate responses

In practice a number of criteria and measures are of interest, e.g., in a queuing situation we may be interested in both waiting time and server utilization, maesured by their means and their 90% quantiles, etc. Though sophisticated statistical tools exist (e.g. Multivariate Analysis of Variance or MANOVA), it is practical to use univariate techniques and to account for the multivariate character by the choice of an appropriate error rate (Bonferroni inequality); see Kleijnen (1975) for more details.

(2) Multiple comparison and ranking procedures

In the first few sections we discussed situations where a number of factors define a great many system variants of potential interest. Relevant techniques are regression analysis and experimental design. A different situation exists, when there are only a few system variants, say, 10, or in general k. These systems may correspond to different queuing disciplines, etc. Multiple comparison procedures (MCP) are suited to situations with k systems (or populations in statistical jargon) and a fixed number of simulation runs (observations) per system. MCP give exact statistical results (controlled α errors) when comparing $k(k-1)/2$ systems with each other, when selecting a subset containing the "best" system (say, highest mean response), etc. Multiple ranking or selection procedures (MRP) have been developed for situations where the number of runs is not fixed, but has to be determined such that the best system can be selected with a prespecified probability of correct selection. Both MCP and MRP are discussed at length in Kleijnen (1975); a recent publication is Dudewicz (1977). At present simulation practitioners have shown little interest in these procedures; the only references we are aware of are Lin (1975) and Vicéns & Schaake (1972).

(3) Statistical input: random numbers, etc.

We have investigated the statistical analysis of the simulation output. On the input side we have the traditional problems of random number generation (multiplicative and shift back generators) and sampling from distributions (including multivariate distributions). References can be found in Kleijnen (1975).

(4) Model validation

Checking whether the model's output conforms with the real world observations can be based on a variety of statistical techniques: t-tests, goodness-of-fit tests, regression analysis, etc. However, this issue involves many more aspects than just statistics; see, e.g., Zeigler (1976).

9. CONCLUSION

Simulation means experimentation, albeit experimentation using a mathematical model instead of the real world. Any experiment requires a sound design. Without such a design even the most sophisticated analysis fails, e.g., if the factors 1 and 2 are changed simultaneously, their separate effects cannot be estimated. Scientific designs such as 2^{k-p} factorials further make it possible to explore the simulation space much more efficiently. The statistical analysis, given the design, should extract as much information from the experiment as is possible, e.g., estimate interactions. Such an analysis can be done systematically by means of a formal metamodel, i.e., a regression model. Moreover, such an analysis shows the limitations of the conclusions. For instance, if the simulation run is too short, so much stochastic noise may be present that instead of an expensive simulation model, a toss of the coin had better been used.

APPENDIX 1: SURVEY OF SIMULATION TYPES

We distinguish the following types of simulation; see also Kleijnen (1976):

(1) Discrete-event models, e.g., queuing systems modeled by a language such as GPSS.Most of the time these models are inherently stochastic, i.e., without the probabilistic character of certain variables the queuing problems would disappear (a scheduling problem would remain).

(2) Time-slicing models of discrete-event systems. It might be convenient to model, say, a highway interchange, by dividing the time-axis into time slices of equal length, and checking which events, if any, occurred.

(3) Difference-equation models, e.g., national econometric and corporate models. Decisions and data for such systems

are of a periodic nature: quarterly, yearly, etc. Usually these models are deterministic.

(4) Difference-equation models for differential equation systems: Forrester's Industrial or System Dynamics using DYNAMO, is a well-known example. Nearly always these models are deterministic.

(5) Digital computer models (by means of difference equations) of continuous phenomena in science and technology: the spontaneous model is formulated in differential equations based on laws of nature known from physics etc. For various reasons a digital computer may be preferred over an analogue/hybrid computer in the solution of the model. Languages such as CSMP and CSSM are used on the digital computer. Note that it is rare that the opposite occurs: an analogue computer (differential equation) used to solve difference equation problems of types 1 through 4.

NOTES

1) In Operations Research, for instance, several surveys have shown that simulation is a most popular technique (together with linear programming and statistical techniques such as regression analysis); see Ledbetter & Cox (1977) for a recent survey and for additional references.
2) Actually the curves in FIG. 1 are no straight lines so that they represent more general formulations than eq. (3.5).
3) These "new" observations might correspond to the "center" of the design ($x_j = 0$ for all factors), in order to check whether pure quadratic effects are zero.
4) In the first eight combinations we use 4 = 12, 5 = 13, 6 = 23 and 7 = 123. In the next eight combinations we switch signs: $x_{i'j} = -x_{ij}$ $(i'=i+1)$ $(i=1,\ldots,8)$.

5) Suppose the individual factors are x_1, x_2,... and we know the signs of the β's, e.g., $\beta_1 \geq 0$ and $\beta_2 \geq 0$. Then x_1 and x_2 can be combined into a single group-factor z_1 with main effect $\gamma_1 = \beta_1 + \beta_2 (\geq 0)$. Hence z_1 is +1 (and -1 respectively) if all its component factors are +1 (and $x_1 = x_2 = -1$ respectively). Execute only two runs (instead of $2^2 = 4$ runs):

   Run 1: $x_1 = -1 \quad x_2 = -1 \rightarrow z_1 = -1$

   Run 2: $x_1 = +1 \quad x_2 = +1 \rightarrow z_2 = +1$

   If responses do not differ significantly, we can conclude that neither x_1 nor x_2 are important, and eliminate x_1 and x_2 from further experimentation. In general, k individual factors x can be combined into g group-factors z which can be tested in a 2^{g-p} fractional factorial design; see Kleijnen (1975b).
6) Split the N design points in two orthogonal blocks, and run one block with common random numbers, and the other block with the antithetic numbers.
7) Notice that n in (7.2) is deterministic, whereas n̲ is stochastic in (7.3). Nevertheless (7.3) gives satisfactory results.
8) When the number of subruns is M, then the variance of the estimated variance is $2\sigma^4/M$ so that the confidence interval for the mean η becomes less stable (but has the same expected length).
9) For the definition of quantiles and percentiles consider $P(x < y) = z$. If z ($0 \leq z \leq 1$) is fixed to, say, 90% then we have to estimate the "quantile" y. If we fix y, then we have to estimate the "percentile" z.

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